Equipartition and Virial theorems in a nonextensive optimal Lagrange multipliers scenario

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Abstract

We revisit some topics of classical thermostatistics from the perspective of the nonextensive optimal Lagrange multipliers (OLM), a recently introduced technique for dealing with the maximization of Tsallis' information measure. It is shown that Equipartition and Virial theorems can be reproduced by Tsallis' nonextensive formalism independently of the value of the nonextensivity index.

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I. INTRODUCTION

Tsallis' thermostatistics (TT) [1–5] is by now recognized as a new paradigm for statistical mechanical considerations. It revolves around the concept of Tsallis' information measure S_q, a generalization of Shannon's one, that depends upon a real index q and becomes Shannon's measure [1] for the particular value $q = 1$.

The Equipartition theorem, first formulated by Boltzmann in 1871, and the Virial one, due to Clausius (1870) [6] are two pillars of classical physics. They were discussed within the TT framework in [7], in terms of the Curado-Tsallis nonextensive normalizing treatment [5], and also in [8], by recourse to escort probabilities [9]. In the present work we are going to revisit these classical subjects in connection with a recently advanced scheme for dealing with Tsallis' thermostatistics [10,11], that seems to yield illuminating insights into classical themes.

Tsallis' thermostatistics involves extremization of Tsallis' entropy by recourse to the celebrated technique of Lagrange. A key TT ingredient is the particular way in which expectation values are computed [9] and, in such a respect, several proposals have been considered during the last ten years [3]. No matter which recipe one chooses (for $q \neq 1$), classical phenomena are always reproduced by TT in the limit $q \to 1$ [3]. Recently, a new algorithm (to be henceforth referred to as the OLM-one) has been advanced to such an extremizing end that diagonalizes the Hessian associated to the Lagrange procedure [10] and yields the optimal Lagrange multipliers associated to the input expectation values. A diagonal Hessian enormously facilitates ascertaining just what kind of extreme the Lagrange method is leading to [10].

A key point in TT considerations is the following one: the entropy constant k is usually identified with Boltzmann's k_B. However, the only certified fact one can be sure of is "$k \to k_B$ for $q \to 1$" [3], which entails that there is room *to choose* $k = k(q)$ *in any suitable way*. It is seen [10] that if one chooses

$$k = k_B \bar{Z}_q^{q-1}, \tag{1}$$

where $\bar{Z}_q$ stands for the partition function, in conjunction with the OLM formalism [10], the classical harmonic oscillator determines a specific heat $C_q = k_B$, so that *the classical Gibbs' result arises without the need to invoke the limit* $q \to 1$. Additionally, this treatment is able i) to reproduce thermodynamics' zero-th law [11], a feat that had eluded previous TT practitioners, and ii) the classical q-independent value for the mean energy of the ideal gas [12]. It is then not unreasonable to conjecture that many other classical results might be obtained by TT without invoking the $q \to 1$ limit.

In the present effort we re-discuss the equipartition theorem and the virial one from an OLM viewpoint. We also revisit the ideal gas problem as an application. More precisely, we perform an OLM treatment of the subject following the canonical ensemble strictures.

II. BRIEF REVIEW OF OLM FORMALISM IN A CLASSICAL SCENARIO

The most general classical treatment requires consideration of the probability density $p(\mathbf{x})$ that maximizes Tsallis' entropy [1,2,13]

$$\frac{S_q}{k} = \frac{1 - \int d\mathbf{x}\ p^q(\mathbf{x})}{q-1}, \tag{2}$$

by recourse to the Lagrange's technique, subject to the foreknowledge of M generalized expectation values [9]

$$\langle\langle O_j \rangle\rangle_q = \frac{\int d\mathbf{x}\ p^q(\mathbf{x}) O_j(\mathbf{x})}{\int d\mathbf{x}\ p^q(\mathbf{x})}, \tag{3}$$

where $O_j(\mathbf{x})$ $(j = 1, \ldots, M)$ denote the M relevant dynamical quantities (the observation level [14]), $q \in \Re$ is Tsallis' nonextensivity index, $\mathbf{x}$ is a phase space element (N particles in a D-dimensional space), and k is the entropy constant, akin to the famous Boltzmann one k_B, employed in the orthodox statistics.

Tsallis' normalized probability distribution [9], is obtained by following the well known MaxEnt route [15]. Instead of effecting the variational treatment of [9], involving $M+1$ Lagrange multipliers λ_j (associated to constraints given by the normalization condition

together with the M equations (3)), the OLM technique follows an alternative path [10] with Lagrange multipliers λ'_j: one maximizes Tsallis' generalized entropy S_q (2) [1,2,13] subject to the *modified* constraints ("centered" generalized expectation values) [1,10]

$$\int d\mathbf{x}\; p(\mathbf{x}) - 1 = 0 \tag{4}$$

$$\int d\mathbf{x}\; p(\mathbf{x})^q \left(O_j(\mathbf{x}) - \langle\langle O_j \rangle\rangle_q\right) = 0. \tag{5}$$

The resulting probability distribution reads [10]

$$p(\mathbf{x}) = \frac{f(\mathbf{x})^{\frac{1}{1-q}}}{\bar{Z}_q}, \tag{6}$$

where

$$\bar{Z}_q = \int d\mathbf{x}\; f(\mathbf{x})^{\frac{1}{1-q}}. \tag{7}$$

and

$$f(\mathbf{x}) = 1 - (1-q) \sum_j^M \lambda'_j \left(O_j(\mathbf{x}) - \langle\langle O_j \rangle\rangle_q\right) \tag{8}$$

is the so-called configurational characteristic.

Although the Tsallis-Mendes-Plastino (TMP) procedure originally devised in [9] overcomes most of the problems posed by the old, unnormalized way of evaluating Tsallis' generalized mean values [9,16], it yields probability distributions that are self-referential, which entails some numerical difficulties. The complementary OLM treatment of [10] surmounts these hardships. Inspection of (6) shows that the self-reference problem has vanished.

One shows in [10] that the relation

$$\int d\mathbf{x}\; p^q(\mathbf{x}) = \bar{Z}_q^{1-q}, \tag{9}$$

valid under TMP, still holds. Eq. (9) allows one to connect the Lagrange multipliers λ_j of the TMP procedure [9] with the corresponding OLM λ'_j via [10]

$$\lambda'_j = \frac{\lambda_j}{\bar{Z}_q^{1-q}}, \tag{10}$$

and to write the entropy as [10]

$$S_q = k \ln_q \bar{Z}_q, \tag{11}$$

where $\ln_q x = (1 - x_q^{1-q})/(q-1)$ has been used.

If now, following [9] we define

$$\ln_q Z'_q = \ln_q \bar{Z}_q - \sum_j \lambda'_j \ \langle\langle O_j \rangle\rangle_q, \tag{12}$$

and additionally use [10]

$$k' = k \ \bar{Z}_q^{1-q}, \tag{13}$$

then [10]

$$\frac{\partial S_q}{\partial \langle\langle O_j \rangle\rangle_q} = k' \lambda'_j \tag{14}$$

$$\frac{\partial}{\partial \lambda'_j} \left(\ln_q Z'_q \right) = - \langle\langle O_j \rangle\rangle_q. \tag{15}$$

Equations (14) and (15) constitute the basic Information Theory relations to build up Statistical Mechanics *à la* Jaynes [15]. Notice that, when k is given by (1), Equation (13) leads to $k' = k_B$ [1].

Remembering that [9]

$$\frac{\partial S_q}{\partial \langle\langle O_j \rangle\rangle_q} = k \lambda_j, \tag{16}$$

one is straightforwardly led to [10]

$$k' \lambda'_j = k \lambda_j, \tag{17}$$

which entails that the intensive variables are identical in both alternative pictures, TMP and OLM [10].

As a special instance of Eq. (17), for the Canonical Ensemble it adopts the appearance

$$k' \beta' = k \beta = \frac{1}{T}. \tag{18}$$

Looking at Eq. (18) one gathers that the temperature T is the same for both sets of Lagrange multipliers.

Before tackling the equipartition theorem, some preliminary results are needed, that we discuss next.

III. NORMALIZATION CONSIDERATIONS

Replacing (6) into (9) we obtain for the partition function the expression

$$\bar{Z}_q = \int d\mathbf{x}\ f(\mathbf{x})^{\frac{q}{1-q}}, \tag{19}$$

and, comparing it to (7), we deduce the (at first sight surprising) relationship

$$\mathcal{D} = \int d\mathbf{x}\ f(\mathbf{x})^{\frac{q}{1-q}} - \int d\mathbf{x}\ f(\mathbf{x})^{\frac{1}{1-q}} = 0, \tag{20}$$

valid for all q. That this is indeed so can also be gathered by first recasting (20) in the form

$$\mathcal{D} = \int d\mathbf{x} \left[f(\mathbf{x})^{\frac{q}{1-q}} \left(1 - f(\mathbf{x})\right)\right], \tag{21}$$

and then using Eq. (8) to obtain

$$\mathcal{D} = (1-q) \sum_j \lambda'_j \int d\mathbf{x} f^{\frac{q}{1-q}} \left(\widehat{O}_j - \left\langle \left\langle \widehat{O}_j \right\rangle \right\rangle_q \right), \tag{22}$$

that, remembering (6), has to vanish identically on account of (5).

We introduce now the factor

$$F(q) \equiv \frac{\int d\mathbf{x} f(\mathbf{x})^{\frac{1}{1-q}}}{\int d\mathbf{x} f(\mathbf{x})^{\frac{q}{1-q}}} = 1, \tag{23}$$

in order to be in a position to use it later on.

It is to be stressed that $F(q) = 1$ only within the so-called "normalized" framework of [9]. If one uses, instead, the Curado-Tsallis normalization [5], this is not so ($F(q) \neq 1$). The OLM formalism does employ the normalized treatment. It must be pointed out that the $F(q) = 1$-result has also been obtained within a purely quantal, Green function scheme by Lenzi, Mendes, and Rajagopal [17].

IV. GENERALIZED EQUIPARTITION AND VIRIAL THEOREMS

In classical statistical physics, a Hamiltonian dynamical system is described by an appropriate phase space probability distribution $p(r_i, p_i)$. Just one assumption will be made on the probability density (PD): that it depend on the phase space variables (r_i, p_i) only through the Hamiltonian $H(r_i, p_i)$.

Tsallis' normalized probability distribution [9] is obtained by maximizing Tsallis' generalized entropy S_q given by Eq. (2), subject to the constraints [1,10]

$$\int d\Omega p(r_i, p_i) = 1 \tag{24}$$

$$\int d\Omega p^q(r_i, p_i) \left(H(r_i, p_i) - \langle\langle H \rangle\rangle_q \right) = 0, \tag{25}$$

where the generalized expectation values [9]

$$\langle\langle H \rangle\rangle_q = \frac{\int d\Omega p^q(r_i, p_i) H(r_i, p_i)}{\int d\Omega p^q(r_i, p_i)} \tag{26}$$

are assumed to be a priori known. They constitute the macroscopic information at hand concerning the system. $d\Omega$ stands for the corresponding phase space volume element

$$d\Omega = (1/(N! h^{DN})) \prod_{i=1}^{DN} dr_i dp_i, \;\; (i = 1 \ldots DN), \tag{27}$$

where h is the linear dimension (i.e. the size) of the elementary cell in phase space, and we assume $\int \prod_{i=1}^{DN} dr_i = V^N$ with V the system's volume.

The resulting probability distribution reads [10]

$$p(r_i, p_i) = \bar{Z}_q^{-1} \left[1 - (1-q)\beta' \left(H(r_i, p_i) - \langle\langle H \rangle\rangle_q \right) \right]^{\frac{1}{1-q}}, \tag{28}$$

where

$$\bar{Z}_q = \int d\Omega \left[1 - (1-q)\beta' \left(H(r_i, p_i) - \langle\langle H \rangle\rangle_q \right) \right]^{\frac{1}{1-q}}. \tag{29}$$

Let $A(q_i,p_i)$ denote a generic dynamical quantity. Its generalized mean value is given by

$$\langle\langle A \rangle\rangle_q = \frac{\int d\Omega \; A(r_i,p_i) \left[1 - \beta'(1-q) \left(H - \langle\langle H \rangle\rangle_q \right) \right]^{\frac{q}{1-q}}}{\int d\Omega \left[1 - \beta'(1-q) \left(H - \langle\langle H \rangle\rangle_q \right) \right]^{\frac{q}{1-q}}}. \tag{30}$$

Let us now assume that our Hamiltonian H can be split into two pieces according to

$$H = g_0 + g \tag{31}$$

where g is a homogeneous function of degree γ of L canonical variables of which, say ν, are generalized coordinates while the remaining ones are $\mu = L - \nu$ generalized momenta

$$g = g(r_1, \ldots, r_\nu, p_1, \ldots, p_\mu), \tag{32}$$

and g_0 does not depend upon these variables. According to Euler's theorem [18] we have

$$\gamma g = \sum_{i=1}^{\nu} r_i(\partial g/\partial r_i) + \sum_{i=1}^{\mu} p_i(\partial g/\partial p_i) \tag{33}$$

so that the generalized mean value of g reads

$$\langle\langle g\rangle\rangle_q = \frac{1}{\gamma}\left[\sum_{i=1}^{\nu}\langle\langle r_i(\partial g/\partial r_i)\rangle\rangle_q + \sum_{i=1}^{\mu}\langle\langle p_i(\partial g/\partial p_i)\rangle\rangle_q\right]. \tag{34}$$

We shall now discuss in some detail one generic term of this equation. Consider

$$\langle\langle r_k(\partial g/\partial r_k)\rangle\rangle_q = \frac{\int d\Omega\; r_k(\partial g/\partial r_k)\left[1 - \beta'(1-q)\left(H - \langle\langle H\rangle\rangle_q\right)\right]^{\frac{q}{1-q}}}{\int d\Omega\left[1 - \beta'(1-q)\left(H - \langle\langle H\rangle\rangle_q\right)\right]^{\frac{q}{1-q}}}, \tag{35}$$

a multi-dimensional ($2DN$) integral. Let us evaluate the integral over r_k ranging between r_a and r_b. These values are given by the well-known Tsallis' cut-off condition [3]: the probability distribution vanishes in those regions of phase space that would make (28) a negative quantity. For the numerator of (35) we have

$$J \equiv \int_{r_a}^{r_b} dr_k\; r_k(\partial g/\partial r_k)\left[1 - \beta'(1-q)\left(H - \langle\langle H\rangle\rangle_q\right)\right]^{\frac{q}{1-q}}, \tag{36}$$

so that

$$\langle\langle r_k(\partial g/\partial r_k)\rangle\rangle_q = \frac{\int \ldots \int J\; dr_1 \ldots dr_{k-1} dr_{k+1} \ldots dp_{DN}}{\int d\Omega\left[1 - \beta'(1-q)\left(H - \langle\langle H\rangle\rangle_q\right)\right]^{\frac{q}{1-q}}}. \tag{37}$$

In order to obtain J we proceed to an integration by parts. To do so we first notice that, on account of Equations (31) and (32)

$$\frac{\partial}{\partial r_k}\left\{\left[1-\beta^{'}(1-q)\left(H-\langle\langle H\rangle\rangle_q\right)\right]^{\frac{1}{1-q}}\right\}=-\beta^{'}\frac{\partial g}{\partial r_k}\left[1-\beta^{'}(1-q)\left(H-\langle\langle H\rangle\rangle_q\right)\right]^{\frac{q}{1-q}}, \quad (38)$$

which, since the integrated part will vanish because of the above mentioned cut-off condition, leads to

$$J=\frac{1}{\beta^{'}}\int dr_k\ \left[1-\beta^{'}(1-q)\left(H-\langle\langle H\rangle\rangle_q\right)\right]^{\frac{1}{1-q}}. \quad (39)$$

Insertion of (39) into (37) yields

$$\langle\langle r_k(\partial g/\partial r_k)\rangle\rangle_q=\frac{1}{\beta^{'}}\frac{\int d\Omega\left[1-\beta^{'}(1-q)\left(H-\langle\langle H\rangle\rangle_q\right)\right]^{\frac{1}{1-q}}}{\int d\Omega\left[1-\beta^{'}(1-q)\left(H-\langle\langle H\rangle\rangle_q\right)\right]^{\frac{q}{1-q}}}, \quad (40)$$

but, on account of (23) one has

$$\langle\langle r_k(\partial g/\partial r_k)\rangle\rangle_q=\frac{1}{\beta^{'}}. \quad (41)$$

It is apparent that each term in the sums appearing in (34) will yield a contribution of the type (41), so that

$$\langle\langle g\rangle\rangle_q=\frac{L}{\gamma\beta^{'}}=\frac{L}{\gamma}k_BT \quad (42)$$

which is a generalized version of the equipartition theorem [6]. We have thus arrived to a new an interesting result. *Contrary to current belief, we see that the classical result is attained, independently of the q-value.*

According to the canonical equations of motion, $\partial H/\partial r_i=-\dot{p}_i$. Hence (41) leads to the statement

$$\left\langle\left\langle\sum_{i=1}^{DN}r_i\dot{p}_i\right\rangle\right\rangle_q=-DNk_BT \quad (43)$$

which is Clausius' virial theorem [6]. Again, *no dependence upon q is to be detected.*

As a simple application, consider now the classical ideal gas. We necessarily reproduce the classical results, by virtue of the above considerations: we deal with N particles confined within a $D-$dimensional box of volume V. Thermodynamical equilibrium at temperature T is assumed. The Hamiltonian is

$$H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + \sum_{i=1}^{N} U_{wall}(\mathbf{r}_i),$$

where U_{wall} is a contribution due to the constraints (walls of the container). The constraint forces come into existence when the gas particles collide with the walls. It thus follows that

$$\sum_{i=1}^{N} \mathbf{r}_i \cdot \frac{\partial H}{\partial \mathbf{r}_i} = -\sum_{i=1}^{N} \mathbf{r}_i \cdot \mathbf{F}_{wall}^{(i)} \tag{44}$$

where $\mathbf{F}_{wall}^{(i)}$ stands for the force on the i-particle due to the walls of the box.

Following now a well-known argument [6], it is possible then to express the last member of the above equation in terms of the volume V and pressure P

$$\begin{aligned} -\sum_{i=1}^{N} \mathbf{r}_i \cdot \mathbf{F}_{wall}^{(i)} &= -P \int_{wall} \mathbf{r} \cdot (-d\mathbf{s}) = P \int_{wall} \mathbf{r} \cdot d\mathbf{s} \\ &= P \int (\nabla \cdot \mathbf{r}) d^3 r = DPV, \end{aligned} \tag{45}$$

where $d\mathbf{s}$ denotes a (vector) surface element of the box in Eq. (44). We get

$$\sum_{i=1}^{N} \mathbf{r}_i \cdot \frac{\partial H}{\partial \mathbf{r}_i} = DPV \tag{46}$$

Now, by taking the canonical average and using the virial theorem (unmodified by the nonextensive scenario) (43), we obtain

$$PV = N k_B T, \tag{47}$$

i.e., the equation of state for the perfect gas. No q-dependence is detected.

For the ideal gas [7,8,12,19], the total energy E is a homogeneous quadratic function ($\gamma = 2$) of DN momenta, which allows one to write, according to (42)

$$\langle\langle H \rangle\rangle_q = \frac{1}{2} D N k_B T. \tag{48}$$

V. CONCLUSIONS

Classical thermostatistics has been the subject of the present effort.

We have tackled some key issues, namely,

- Virial theorem,
- Equipartition theorem,
- Equation of state of the ideal gas,

and shown that they are, contrary to present belief, reproduced by Tsallis' thermostatistics *independently of the value adopted by the index* q. The present work lends further credence to the hypothesis that most important classical statistical results might be reproduced by Tsallis' thermostatistics for all q-values.

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